Ethyl heptanoate
106-30-9 | DTXSID1040112

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		**Training (75%)**		**Test (25%)**	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.12e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.23e-01

Confidence level: 8.54e-01

Nearest Neighbors from the Training Set

Image not found
Butyl butyrate
Measured: 1.06e-11
Predicted: 1.06e-11

Image not found
2-Ethoxyethyl isobutyrate
Measured: 1.35e-11
Predicted: 1.28e-11

Image not found
Butanoic acid, propyl ester
Measured: 7.41e-12
Predicted: 6.98e-12

Image not found
Pentyl acetate
Measured: 7.55e-12
Predicted: 6.38e-12

Image not found
Ethyl 3-ethoxypropionate
Measured: 2.29e-11
Predicted: 1.63e-11